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Welcome to STN International! Enter x:x

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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* * * * * * * *
                     Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
NEWS
        Feb 24
                 PCTGEN now available on STN
     3
NEWS
        Feb 24
                 TEMA now available on STN
        Feb 26 NTIS now allows simultaneous left and right truncation
NEWS
      5
NEWS
        Feb 26
                PCTFULL now contains images
      6
                 SDI PACKAGE for monthly delivery of multifile SDI results
NEWS
      7
         Mar 04
         Mar 24
                 PATDPAFULL now available on STN
NEWS
      8
NEWS
         Mar 24
                 Additional information for trade-named substances without
      9
                 structures available in REGISTRY
         Apr 11
                 Display formats in DGENE enhanced
NEWS 10
NEWS 11
         Apr 14
                 MEDLINE Reload
                 Polymer searching in REGISTRY enhanced
NEWS 12
         Apr 17
                 Indexing from 1937 to 1946 added to records in CA/CAPLUS
NEWS 13
         AUG 15
NEWS 14
                 New current-awareness alert (SDI) frequency in
         Apr 21
                 WPIDS/WPINDEX/WPIX
NEWS 15
                 RDISCLOSURE now available on STN
         Apr 28
                 Pharmacokinetic information and systematic chemical names
NEWS 16
         May 05
                 added to PHAR
NEWS 17
         May 15
                 MEDLINE file segment of TOXCENTER reloaded
                 Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 18
         May 15
NEWS 19
         May 19
                 Simultaneous left and right truncation added to WSCA
NEWS 20
                 RAPRA enhanced with new search field, simultaneous left and
         May 19
                 right truncation
                 Simultaneous left and right truncation added to CBNB
NEWS 21
         Jun 06
NEWS 22
         Jun 06
                 PASCAL enhanced with additional data
NEWS 23
                 2003 edition of the FSTA Thesaurus is now available
         Jun 20
         Jun 25
                 HSDB has been reloaded
NEWS 24
NEWS 25
         Jul 16
                 Data from 1960-1976 added to RDISCLOSURE
NEWS 26
                 Identification of STN records implemented
         Jul 21
NEWS 27
         Jul 21
                 Polymer class term count added to REGISTRY
NEWS 28
         Jul 22
                 INPADOC: Basic index (/BI) enhanced; Simultaneous Left and
                 Right Truncation available
NEWS 29
         AUG 05
                 New pricing for EUROPATFULL and PCTFULL effective
                 August 1, 2003
                 Field Availability (/FA) field enhanced in BEILSTEIN
         AUG 13
NEWS 30
NEWS 31
         AUG 15
                 PATDPAFULL: one FREE connect hour, per account, in
                 September 2003
                 PCTGEN: one FREE connect hour, per account, in
         AUG 15
NEWS 32
                 September 2003
NEWS 33
         AUG 15
                 RDISCLOSURE: one FREE connect hour, per account, in
                 September 2003
NEWS 34
         AUG 15
                 TEMA: one FREE connect hour, per account, in
```

September 2003

NEWS 35 AUG 18 Data available for download as a PDF in RDISCLOSURE NEWS 36 AUG 18 Simultaneous left and right truncation added to PASCAL

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003

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NEWS WWW CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 14:34:32 ON 18 AUG 2003

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:34:42 ON 18 AUG 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 15 AUG 2003 HIGHEST RN 567484-39-3 DICTIONARY FILE UPDATES: 15 AUG 2003 HIGHEST RN 567484-39-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

Uploading 10173277.str

L1 STRUCTURE UPLOADED

Uploading 10018842.str

Kamal Saeed

L2 STRUCTURE UPLOADED

=> d

L2 HAS NO ANSWERS

L2 STI

Structure attributes must be viewed using STN Express query preparation.

=> s 12 full

FULL SEARCH INITIATED 14:36:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS

A TO TO A CO

1 ANSWERS

SEARCH TIME: 00.00.01

L3 1 SEA SSS FUL L2

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 148.95 149.16

FULL ESTIMATED COST

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FILE COVERS 1907 - 18 Aug 2003 VOL 139 ISS 8 FILE LAST UPDATED: 17 Aug 2003 (20030817/ED)

This file contains CAS Registry Numbers for easy and accurate

Kamal Saeed

substance identification.

=> s 13

=> s 13 L4 1 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:584508 CAPLUS
DOCUMENT NUMBER: 135:318698
TITLE: 135:318698
FMc-POAC: ([9-fluorenylmethyloxycarbonyl]-2,2,5,5tetramethylpyrrolidine-N-oxyl-3-amino-4-oarboxylic
acid]: a novel protected spin labeled .beta.-amino
acid for peptide and protein chemistry
Tominaga, Mineko; Barbosa, Simone Reis; Poletti,

AUTHOR(S): Erick

AUTHOR(S): Tomknaga, Mineko; Barbosa, Simone Reis; Poletti,
Erick

Pernando; Zukerman-Schpector, Julio; Marchetto,
Reinaldo; Schreier, Shirley; Palva, Antonio Cechelli
Mattos Mattos; Nakaie, Clovis Ryuichi
Department of Biophysics, Universidade Federal de Sao
Paulo, Sao Paulo, 04044-020, Brazil
Chemical & Pharmaceutical Bulletin (2001), 49(8),
1027-1029
COEDN: CPBTAL; ISSN: 0009-2363
PHARMACHURAL BUILDEN
LANGUAGE: Pharmaceutical Society of Japan
Journal
LANGUAGE: English
AB The stable free radical 2,26,6-tetramethylpiperidine-N-oxyl-4-amino-4carboxylic acid (TOAC) is the only spin labeled amino acid that has been
used to date to successfully label peptide sequences for structural
studies. However, severe difficulty in coupling it with an amino acid

studies. However, severe difficulty in coupling it with an amino acid has been the most serious shortcoming of this paramagnetic marker. The present report introduces the alternative beta.-amino acid 2,2,5,5-tetramethylpyrrolidine-N-oxyl-3-amino-4-carboxylic acid (POAC), potentially useful in peptide and protein chem. X-ray diffraction measurements of POAC in cryst. and bulk samples revealed that it consists only of the trans conformer. The amine function of POAC was protected with 9-fluorenylmethyloxycarbonyl (Fmoc), such that Fmoc-POAC can be used in peptide synthesis. Por example, vasoactive octapeptide angiotensin II (AII; DRVYIHPF) was synthesized by replacing Pro7 with POAC. The reaction of Pmoc-POAC with the peptidyl resin occurred smoothly, and the coupling of the subsequent amino acid showed a much faster reaction than when compared with TOAC. POAC7-AII was obtained in a good yield, demonstrating that, in addn. to TOAC, POAC is a convenient amino acid for the synthesis of spin labeled peptide analogs.

IT 367493-80-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of Fmoc-POAC as a protected, spin labeled .beta.-amino acid for incorporation into angiotensin II)

for

incorporation into angiotensin II) 367493-88-7 CAPLUS 1-Pyrrolidinyloxy, 3-carboxy-4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2,2,5,5-tetramethyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 24 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

TAL
ION
.53
TAL
ION
.65

FILE 'REGISTRY' ENTERED AT 14:37:30 ON 18 AUG 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 15 AUG 2003 HIGHEST RN 567484-39-3 DICTIONARY FILE UPDATES: 15 AUG 2003 HIGHEST RN 567484-39-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10018842.str

L5 STRUCTURE UPLOADED

=> d L5 HAS NO ANSWERS L5 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 15 full

FULL SEARCH INITIATED 14:38:00 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 242 TO ITERATE

100.0% PROCESSED 242 ITERATIONS 4 ANSWERS

SEARCH TIME: 00.00.01

4 SEA SSS FUL L5

=> file caplus

SINCE FILE TOTAL ENTRY SESSION 148.15 302.68 COST IN U.S. DOLLARS FULL ESTIMATED COST

TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -0.65

FILE 'CAPLUS' ENTERED AT 14:38:08 ON 18 AUG 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 18 Aug 2003 VOL 139 ISS 8 FILE LAST UPDATED: 17 Aug 2003 (20030817/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16

L7 11 L6

=> d ibib abshitstr tot 'ABSHITSTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB

ALL ----- BIB, AB, IND, RE

APPS ----- AI, PRAI

BIB ----- AN, plus Bibliographic Data and PI table (default) CAN ----- List of CA abstract numbers without answer numbers

```
CBIB ----- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN) STD ----- BIB, IPC, and NCL
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
             containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
             its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
FHITSTR ---- First HIT RN, its text modification, its CA index name, and
             its structure diagram
FHITSEQ ---- First HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs
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=> d ibib abs hitstr tot

```
L7 ANSWER 1 OF 11
ACCESSION NUMBER:
DOCUMENT NUMBER:
TITLE:
SINVENTOR(S):
PATENT ASSIGNEE(S):
BOURCE:
DOCUMENT TYPE:

COPYRIGHT 2003 ACS on STN
2003:242180 CAPLUS
138:271975
Preparation of .beta.-peptides in method for delivery of molecules to intracellular targets
Gellman, Samuel H.; Umezawa, Naoki; Gelman, Michael A.; Raines, Ronald T.; Potocky, Terra
PATENT ASSIGNEE(S):
DOCUMENT TYPE:

COPEN: PIXXD2
Patent
            DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                                                                                                                                                                               KIND DATE
PATENT NO. KIND DATE

WO 2003024477 A1 20030327 W0 2002-US29568 20020918

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EG, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, ND, MG, MK, MN, MM, MX, NO, NZ, CM, PH, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, GG, CI, CM, GA, GM, GQ, GW, ML, MR, NS, MS, CB, TD, TG

US 2003119189 A1 20030626 US 2002-246441 20020918

PRIORITY APPINA INFO: US AMARPAT 138:271975 2010-323512 P 20010918

OTHER SOURCE(S): MARRPAT 138:271975 A1 2001-323512 P 20010918

OTHER SOURCE(S): MARRPAT 138:271975 A1 2001-323512 P 20010918

CAS AB Disclosed are beta-peptides and beta-peptide conjugates that are capable of diffusing or otherwise being transported across the cell membranes of living eldus, 1 least six of which are preferably beta-3-homographine residues. When pharmacol-active agents are conjugated to these types of beta-peptides, the resulting conjugates (also disclosed) are also capable of diffusing or otherwise being transported across the cell membranes of living cells, including mammalian
                                                        PATENT NO.
                                                                                                                                                                                                                                                                                                                                                                                                                                        APPLICATION NO. DATE
                                                             cells. The examples include the synthesis of cyclohexyl-contg.
.beta.-amino acids and the soln.-phase synthesis of a .beta.-peptide
                                                contg. alternating residues of unsubstituted cyclohexane rings and amino-substituted cyclohexane rings.
267230-44-4P.
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn of beta-peptides in method for delivery of mols. to content to the content of the co
       Absolute stereochemistry. Rotation (-).
```

```
ANSWER 2 OF 11
CAPLUS COPYRIGHT 2003 ACS on STN
2003:76804 CAPLUS
E: 138:137596
Antimicrobial compositions containing .beta.-amino acid oligomers
CHOR(S): Gellman, Samuel H.; Weisblum, Bernard; Porter, Emilie Ann; Wang, Xifang
Wisconsin Alumni Research Foundation, USA
PCT Int. Appl., 101 pp.
CODEN: PIXXD2
MENT TYPE: Patent
UNGE: English
ACCESSION NUMBER:
DOCUMENT NUMBER:
DOCUMENTITLE:
PATENT ASSIGNEE(S):
SOURCE:
DOCUMENT TYPE:
LANGUAGE:
                                                                         English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
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PATENT NO.
                                                                                                                                                                    KIND DATE
                                                                                                                                                                                                                                                                                                                               APPLICATION NO. DATE
### PATENT NO. KIND DATE APPLICATION NO. DATE

### O 2003008439 Al 20030130 W0 2001-US22801 20010718

W: AB, AG, AL, AM, AT, AU, AZ, BA, BB, BB, BR, BY, BZ, CA, CH, CN, CO, CR, CU, C2, DE, DK, DM, DZ, EG, EE, ES, FI, GB, GD, GB, GH, GM, HR, HU, ID, II, IN, IS, JF, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, MZ, PL, FT, RO, RU, SD, SE, SG, SI, SK, SI, TJ, TM, TR, TT, TZ, UA, UG, UZ, VM, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SI, SZ, TZ, UG, ZW, AT, BB, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, FT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GM, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPIN. INFO: W0 2001-US22801 20010718

AB Disclosed are antimicrobial compns. contg. .beta.-peptides and methods of inhibiting microbial growth in mammals using the compns. The .beta.-peptides present in the compns. contain ring structures in the peptide backbone which limit the conformational flexibility of the peptides. Commods. W-INICH/XICH/YICO]D-Z [D is an integer > 6: W is H or peptides. AM of the compons. Contain ring structures in the peptides. Commods. W-INICH/XICH/YICO]D-Z [D is an integer > 6: W is H or peptides. AM of the compons. Contain ring structures in the peptides. Commods. W-INICH/XICH/YICO]D-Z [D is an integer > 6: W is H or Description.
                                        de hackbone. Compds. W-[NHCH(X)CH(Y)CO]p-Z [p is an integer > 6; W is H or an amino-terminal capping group; Z is OH or a carboxy-terminal capping group; X = H, alk(en)(yn)yl, mono- or bicyclic (hetero)aryl, (CH2)n+1-functional group (n = 0-6), etc.; Y = H, alk(en)(yn)yl, mono- or bicyclic (hetero)aryl, (CH2)n-functional group, etc.; Or X-CHCH-Y are (un)substituted cycloalk(en)yl or heterocyclic rings] are claimed. Oligomers contg. (R,R)-trans-2-aminocyclopentanecarboxylic acid (ACPC)
                                          (R,R)-trans-4-aminopyrrolidine-3-carboxylic acid (APC) residues of
                                   NIA

AC-ACPC-ACPC-(APC-APC-APC-APC-APC) n-NH2 [n = 1, 2, or 3 (.beta.17); in protonated forms] were prepd. and evaluated for antimicrobial and non-hemolytic activities. The antibacterial activity of .beta.17 is comparable to that of magainin.

267230-44-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of .beta.-amino acid oligomers for antimicrobial compns.)

267230-44-4 CAPLUS

1,3-Pyrrolidinedicarboxylic acid, 4-[[9H-fluoren-9-ylmethoxylcarbonyl]amino]-, 1-(1,1-dimethylethyl) ester, (3R,4S)- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry. Rotation (-).

ANSWER 1 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT: THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
137:325636
Synthesis and 12-Helical Secondary Structure of
.beta.-Peptides Containing (2R, 3R)-Aminoproline
Porter, Emilie A.; Wang, Xifang; Schmitt, Margaret

CORPORATE SOURCE:

Gellman, Samuel H.

Department of Chemistry, University of Wisconsin,
Madison, WI, 53706, USA
Organic Letters (2002), 4(19), 3317-3319
CODEN: ORLEFT; ISSN: 1523-7060
American Chemical Society
Journal
English
CASREACT 137:325636 SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

(2R,3R)-Aminoproline, a pyrrolidine-based .beta.-amino acid, was synthesized and incorporated into hexa-.beta.-peptide I. This residue confers water soly, when the ring nitrogen is protonated and allows for 12-helix formation in aq. soln. CD spectra display the 12-helical signature, which was confirmed by 2D NMR anal. 267330-44-4

267230-44-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aminoproline-contg. .beta.-peptides and their helical
secondary structure anal. by CD and NNR)
267230-44-4 CAPLUS
1,3-Pyrrolidinedicarboxylic acid, 4-[[(9H-fluoren-9ylmethoxylycarbonyl]amino]-, 1-(1,1-dimethylethyl) ester, (3R,4S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

ANSWER 4 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN SSION NUMBER: 2002:241368 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: TITLE:

LUS COPYRIGHT 2003 ACS on STN 2002:241368 CAPLUS 136:263480 Preparation of .beta.-amino acids and .beta.-polypeptides Gellman, Samuel H.; Appella, Daniel H.; Lee, Hee-Seung; Leplae, Paul; Porter, Emilie; Wang, INVENTOR(S):

Woll, Matthew PATENT ASSIGNEE (S):

Woll, Matthew
USA
U.S. Pat. Appl. Publ., 48 pp., Cont.-in-part of U.S.
Ser. No. 464,212.
CODEN: USEXCO
Patent
English
2 SOURCE:

DOCUMENT TYPE:

PATENT NO. KIND DATE APPLICATION NO. DATE

monomers.

The 1H NMR and CD spectra of polypeptides, e.g., the dimer and hexamer of trans-2-aminocyclohexanecarboxylic acid, are shown. Methods of generating combinatorial libraries of polypeptides contg. the .beta.-peptide

dues
are given.
267230-44-4P
RL: SPN (8ynthetic preparation); PREF (Preparation)
(prepn. of .beta.-amino acids and .beta.-polypeptides)
267230-44-4 CAPLUS
1,3-Pyrrolidinedicarboxylic acid, 4-[[[9H-fluoren-9ylmethoxylcarbonyl]amino]-, 1-(1,1-dimethylethyl) ester, (3R,4S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

(Continued) ANSWER 3 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN

THERE ARE 38 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 4 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

```
L7 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:185719 CAPLUS
DOCUMENT NUMBER: 136:248076
Oligomers and polymers of di-substituted cyclic imino carboxylic acids
Gellman, Samuel H.; Huck, Bayard R.
USA
USA
U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S.
Ser. No. 592,756.
                                                                                 CODEN: USXXCO
  DOCUMENT TYPE:
                                                                                 English
  FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:
                                                                       KIND DATE
                 PATENT NO.
                                                                                                                                           APPLICATION NO. DATE
                                                                         A1
A2
A3
                 US 2002032334
                                                                                          20020314
                                                                                                                                           US 2001-883579 20010618
WO 2002-US19050 20020617
                 WO 2002102983
WO 2002102983
                                                                                          20021227
20030515
                                        102983 A3 20030515
AE, AG, AL, MM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, II, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LS, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TM, TR, TT, CUA, UG, UG, UG, UG, UG, UG, UG, MA, AZ, BY, KG, KZ, MD, RU, TJ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
                              W:
TM

RW: GH, GM, KE, LS, NW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, LE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, GF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG PRIORITY APPLN. INFO.:

US 1999-138972P P 19990614

US 2000-592756 A2 20000613

Disclosed are cyclic imino oligomers and polymers comprising pyrrolidine or piperidine groups. Also disclosed are combinatorial libraries and arrays of the cyclic imino compds. Oligomers of benzyl

TY 26723-44-4P

RL: IMF (Industrial manufacture); RCT (Reactant); PREF (Preparation);
 TM
                (Reactant or reagent)
(Oligomers and polymers of di-substituted cyclic imino carboxylic acids)
267230-44-4 CAPLUS
                26/230-44-4 CAPLOS
1,3-Pyrrolidinedicarboxylic acid, 4-[[(9H-fluoren-9-
ylmethoxy]carbonyl]amino]-, 1-(1,1-dimethylethyl) ester, (3R,4S)- (9CI)
(CA INDEX NAME)
 Absolute stereochemistry, Rotation (-).
```

ANSWER 6 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) COoH REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN

CO2H

(Continued)

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ANSWER 6 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN
SSION NUMBER: 2001:594508 CAPLUS
E: Finoc-POAC: [(9-fluorenyimethyloxycarbonyl)-2,2,5,5-tetramethylpyrrolidine-N-oxyl-3-amino-4-carboxylic acid]: a novel protected spin labeled .beta.-amino acid for peptide and protein chemistry
Tominaga, Mineko; Barbosa, Simone Reis; Poletti,
 AUTHOR(S):
Erick
                                                                                                 Fernando: Zukerman-Schpector, Julio: Marchetto,
Reinaldo: Schreier, Shirley: Paiva, Antonio Cechelli
Mattos Mattos: Nakaie, Clovis Ryuichi
Department of Biophysics, Universidade Federal de Sao
Paulo, Sao Paulo, 04044-020, Brazil
Chemical & Pharmaceutical Bulletin (2001), 49(8),
1027-1029
CODEN: CPBTAL; ISSN: 0009-2363
Pharmaceutical Society of Japan
Journal
CORPORATE SOURCE:
 SOURCE .
 PUBLISHER:
PUBLISHER: FINAL MACHINE FOR TYPE: Journal LANGUAGE: Brightsh B The stable free radical 2,2,6,6-tetramethylpiperidine-N-oxyl-4-amino-4-carboxylic acid (TOAC) is the only spin labeled amino acid that has been used to date to successfully label peptide sequences for structural studies. However, severe difficulty in coupling lt with an amino acid
                 been the most serious shortcoming of this paramagnetic marker. The present report introduces the alternative .beta.-amino acid 2,2,5,5-tetramethylpyrrolidine-N-oxyl-3-amino-4-carboxylic acid (POAC), potentially useful in peptide and protein chem. X-ray diffraction measurements of POAC in cryst. and bulk samples revealed that it consists only of the trans conformer. The amine function of POAC was protected with 9-fluorenylmethyloxycarbonyl (Fmoc), such that Emoc-POAC can be used in peptide synthesis. For example, vascactive octapeptide angiotensin II (AII; DRVYIHPF) was synthesized by replacing Pro7 with POAC. The tion
                  tion
of Fmoc-POAC with the peptidyl resin occurred smoothly, and the coupling
of the subsequent amino acid showed a much faster reaction than when
compared with TOAC. POACTAII was obtained in a good yield,
nstrating
that, in addn. to TOAC, POAC is a convenient amino acid for the synthesis
of spin labeled peptide analogs.
367493-88-79
                    J57493-88-7P
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
IT
                               eactant or reagent)
(prepn. of Fmoc-POAC as a protected, spin labeled .beta.-amino acid
for
                   incorporation into angiotensin II) 367(93-88-7 CAPIUS 1-Pyrrolidinyloxy, 3-carboxy-4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2,2,5,5-tetramethyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)
```

Relative stereochemistry.

ACCESSION NUMBER: DOCUMENT NUMBER: TITLE:

L7 ANSWER 7 OF 11
ACCESSION NUMBER:
DOCUMENT NUMBER:
157:1242486
Diversity in Short .beta.-Peptide 12-Helices:
High-Resolution Structural Analysis in Aqueous
Solution of a Hexamer Containing Sulfonylated
Pyrrolidine Residues
Lee, Hee-Seung; Syud, Faisal A.; Wang, Xifang;
Gellman, Samuel H.
Department of Chemistry, University of Wisconsin,
Madison, WI, 53706, USA
Journal of the American Chemical Society (2001),
123(31), 7721-7722
CODEN: JACSAT: ISSN: 0002-7863
American Chemical Society
Journal
LANGUAGE:
English

$$\bigcap_{N \in \mathbb{N}} \bigcap_{N \in \mathbb{N}} \bigcap_{$$

sulfonylaminopyrrolidinecarboxylate) 359894-99-8 CAPLUS

RN 359894-99-8 CAPIUS
CN 3-Pyrrolidinecarboxylic acid,
4-[[(9H-fluoren-9-ylmethoxy|carbonyl]amino]1-[(4-methoxyphenyl)sulfonyl]-, (3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 8 OF 11
ACCESSION NUMBER: 2001:270984 CAPLUS
DOCUMENT NUMBER: 135:76741
ATTILE: 2001:270984 CAPLUS
135:76741
ATTILE: 315:76741
ATTILE: 315:76741
ATTILE: 315:76741
ATTILE: 316:76741
A

SOURCE: 3597-3599

CODEN: JOCEAN; ISSN: 0022-3263 American Chemical Society Journal English CASREACT 135:76741 PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GT

FmocN согн CO2H COSEt H₂N

The enantiomers of a protected trans-4-amino-3-pyrrolidinecarboxylic acid I, used in the prepn. of helical .beta.-peptides, are prepd. stereoselectively in 2 stages from Et N-Boc-3-oxopyrrolidinecarboxylate II. The key step of the synthesis is the stereoselective reductive amthation of II with nonracemic .alpha.-methylbenzylamines to give the trans-.beta.-amino acid stereoselectively and in nonracemic form. E.g.,

was stirred in abs. ethanol with 2 equiv. $\{R\}^{-}(+)^-$.alpha.—methylbenzylamine in the presence of glacial acetic acid for 3 h; 4 equiv

methylbenzylamine in the presence of glacial acetic acid for 3 h; 4

1v.

sodium cyanoborohydride was added and the mixt. stirred at 75.degree. for
14 h (with caution due to possible HCN evolution); concn. followed by
treatment with 4N HCl in dioxane and stirring for 3 h at room temp, gave
the nonracemic methylbenzylaminopyrrolidinecarboxylate III as its
monohydrochloride in 38t yield. E.g., III was dissolved in
methanol/THF/water and stirred at 0.degree. with excess lithium hydroxide
for 3 h; neutralization with 1N aq. HCl and evapn, gave the free acid
hydrochloride as a white solid; the white solid was then dissolved in
acetone/H2O and reacted with Pmoc-Osu and sodium bloarbonate at 0.degree.
for 1 h and at room telm, overnight; after workup, (-)-(35,4R)-I was
isolated in 728 yield hydrochloride and solid was then dissolved in
(Stynthetic preparation); PREP (Preparation)
(Stereoselectic acetocylate derivs. by reductive amination of an
aminopyriolimecarboxylate derivs. by reductive amination of an
acopyriolimedicarboxylate with .alpha-methylbenzylamines)
(20 13-Py-91 didinedicarboxylic acid, 4-[(9H-fluoren-9ylmethoxy)carbonyl]amino]-, 1-(1,1-dimethylethyl) ester, (3R,4S)- (9CI)
(CA INDEX NAME)

Kamal Saeed

ANSWER 7 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

44

REFERENCE COUNT: THIS

THERE ARE 44 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L7 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry. Rotation (-).

346610-79-5 CAPLUS 1,3-Pyrrolidinedicarboxylic acid, 4-[([9H-fluoren-9-ylmethoxyl)carbonyl]amino]-, 1-(1,1-dimethylethyl) ester, (3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

```
L7 ANSWER 9 OF 11
ACCESSION NUMBER:
DOCUMENT NUMBER:
TITLE:
LNVENTOR(S):
Gellman, Samuel H.; Huck, Bayard R.; Richards,
  INVENTOR(S):
Michele
                                                                          R. wisconsin Alumni Research Foundation, USA PCT Int. Appl., 59 pp. CODEN: PIXXD2 Patent
 PATENT ASSIGNEE(S):
SOURCE:
  DOCUMENT TYPE:
 LANGUAGE: FACENT ENGLISH FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:
                                                                                                                               APPLICATION NO. DATE
R: AT, BE, CH, DE, DK, ES, FK, GB, GK, TY, LL, LD, NL, SE, AC, FI, DZ 2003502316 T2 20030121 JP 2001-503834 20000613

RITY APPLN. INFO.: US 1999-138972P P 19990614

Compds. X-(A)n-Y, [n is an integer > 1; X or Y is H, OH, an amino- or carboxy-terminal capping group, or salts; A represents substituted 3-piperidinecarboxylic acid, 3-piperazinecarboxylic acid or 3-pyrrolidinecarboxylic acid attached at the N atom and carbonyl group were prepd. for generating combinatorial libraries. The preferred conformations of the prepd. oligomers were detd. by CD and mol. modeling. Thus, Boc([s]-FCA]3-OCH2Ph (Boc = tert-butoxycarbonyl, FCA = 3-pyrrolidinecarboxylic acid) was prepd. by std. peptide coupling in
  soln
                and its CD suggests distinct secondary structure. 267230-44-4P
               267230-44-49

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation of unnatural peptide-like cyclic imino
carboxylic acid oligomers)
267230-44-4 CAPLUS
1,3-Pyrrolidinedicarboxylic acid, 4-{[(9H-fluoren-9-
ylmethoxyl)carbonyl]amino}-, 1-(1,1-dimethylethyl) ester, (3R,48)- (9CI)
(CA INDEX NAME)
```

L7 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 2000:307139 CAPLUS 2000:307139 132:322149 DOCUMENT NUMBER: TITLE: 132:322149
Preparation of .beta.-polypeptide foldamers of
well-defined secondary structure
Gellman, Samuel H.; Appella, Daniel H.; Christianson,
Laurte A.; Klein, Daniel A.; Krauthauser, Susanne;
Chung, Yong Jun; Wang, Xifang
Wisconsin Alumni Research Foundation, USA
U.S. 42 pp.
CODEN: USAXAM INVENTOR (S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: Patent English 2 FAMILY ACC. NUM. COUNT: PATENT INFORMATION: A 20000509 A1 20020328 APPLICATION NO. DATE PATENT NO. ### APPLICATION NO. DATE

US 6060585 A 20000509 US 1998-34509 19980304
US 2002037997 A1 20020328 US 2001-833496 20010411
RITY APPIN. INFO:

US 1998-34509 A3 19980304
US 1998-34509 A3 19980304
US 1999-464212 A2 19991215

Polypeptides { (NHCHXCHYCO)n-Z-(NHCHXCHYCO)p)m [Z is a single bond, a prolyl-qlycolic acid linkage, or a di-nipecotic acid residue; when Z is a single bond, X and Y together with the carbon atoms to which they are bonded, define (un)substituted cycloalkyl, cycloalkenyl or a heterocyclic ring having one or more nitrogen atoms; when Z is not a single bond, X PRIORITY APPLN, INFO.:

ring having one or more nitrogen atoms; when Z is not a single bond, X Y are as defined above or independently selected form hydroxy, alkyl, alkonyl, alkynyl, hydroxy- or aminoalkyl, alkoya, alkoyalkyl, amino, carboxamido, sulfonamido, cyano, mono- or bicyclic aryl or heteroaryl, etc.; m, n, and p are pos. integers] were prepd. The .beta.-peptides adopt stable helical and sheet structures in both the solid state and in soln. The IH NNR and CD spectra of polypeptides, e.g., the dimer and hexamer of trans-2-aminocyclohoxanecarboxylic acid, are shown. Method of generating combinatorial libraries of peptides contg. .beta.-peptide residues and the libraries formed thereby are disclosed.

267230-44-49
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of .beta.-polypeptide foldamers of well-defined secondary structure)
267230-44-4 CAPLUS
1,3-Fyrrolidinedicarboxylic acid, 4-[[(9H-fluoren-9-ylmethoxylcarbonyl]aminol-, 1-(1,1-dimethylethyl) ester, (3R,4S)- (9CI) (CA INDEX NAME) and Method of

Absolute stereochemistry. Rotation (-).

ANSWER 9 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

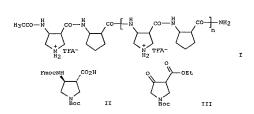
ANSWER 10 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT: THIS THERE ARE 17 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Absolute stereochemistry. Rotation (-).

L7 ANSWER 11 OF 11
ACCESSION NUMBER:
DOCUMENT NUMBER:
137:89780
12-Helix formation in aqueous solution with short
.beta.-peptides containing pyrrolidine-based residues
Wang, Xifang; Espinosa, Juan F.; Gellman, Samuel H.
Department of Chemistry, University of Wisconsin,
Madison, WI, 53706, USA
Journal of the American Chemical Society (2000),
122(19), 4821-4822
CODEN: JACSAT; ISSN: 0002-7863
American Chemical Society
Journal
LANGUAGE:
English
GI

PUBLISHER: DOCUMENT TYPE: LANGUAGE: GI



The design, synthesis and conformational anal. of a set of .beta.-amino acid oligomers (".beta.-peptides") I (n = 1-3; TFA = trifluoroacetate) were presented. One of the .beta.-amino acids, protected 3-aminopyrrolidine-4-carboxylate II, was synthesized in an enantiopure form from .beta.-ketoester III. I was synthesized from the .beta.-amino acids II and (R,R)-2-aminocyclopentanecarboxylate using solid-phase methodol. with Rink amide resin, Fmoc/Boc protection and PyBoP as the coupling agent; after REDC purifications, I was isolated as a trifluoroacetate salt. Using NMR and CD, detailed conformational anal.

I (n=2) was provided.

267230-44-4P
RL: RCT (Reactant); SFN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of enanticopure aminopyrrolidinecarboxylate)
267230-44-4 CAPLUS
1,3-Pyrrolidinedicarboxylic acid, 4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, 1-(1,1-dimethylethyl) ester, (3R,4S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

ANSWER 11 OF 11 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT: THIS

38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

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ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

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FULL ESTIMATED COST

SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION
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